PumpKin: A tool to find principal pathways in plasma chemical models

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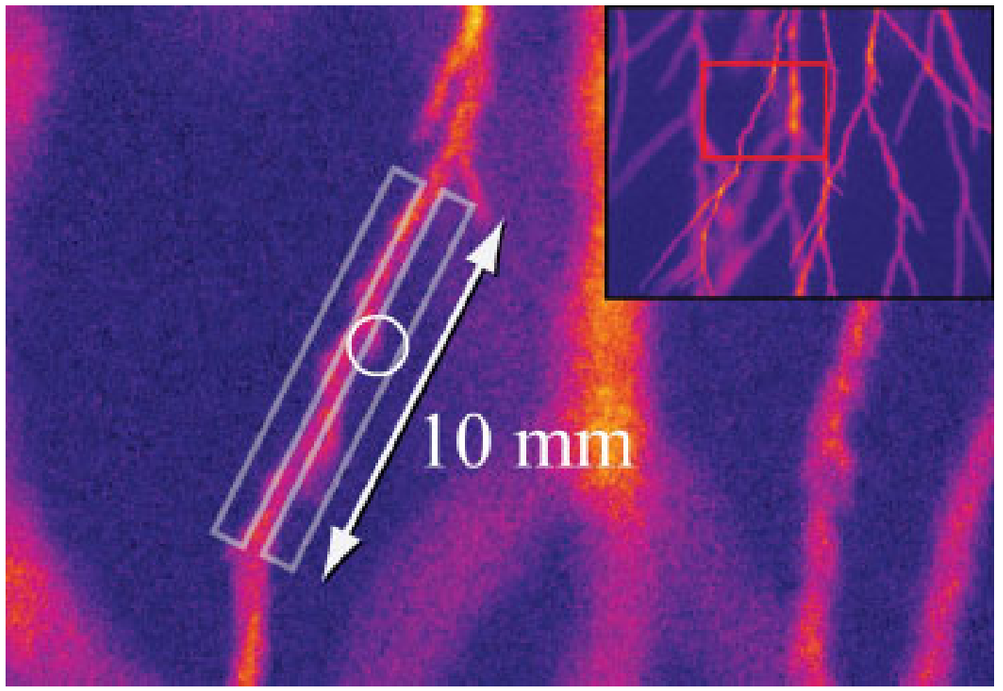
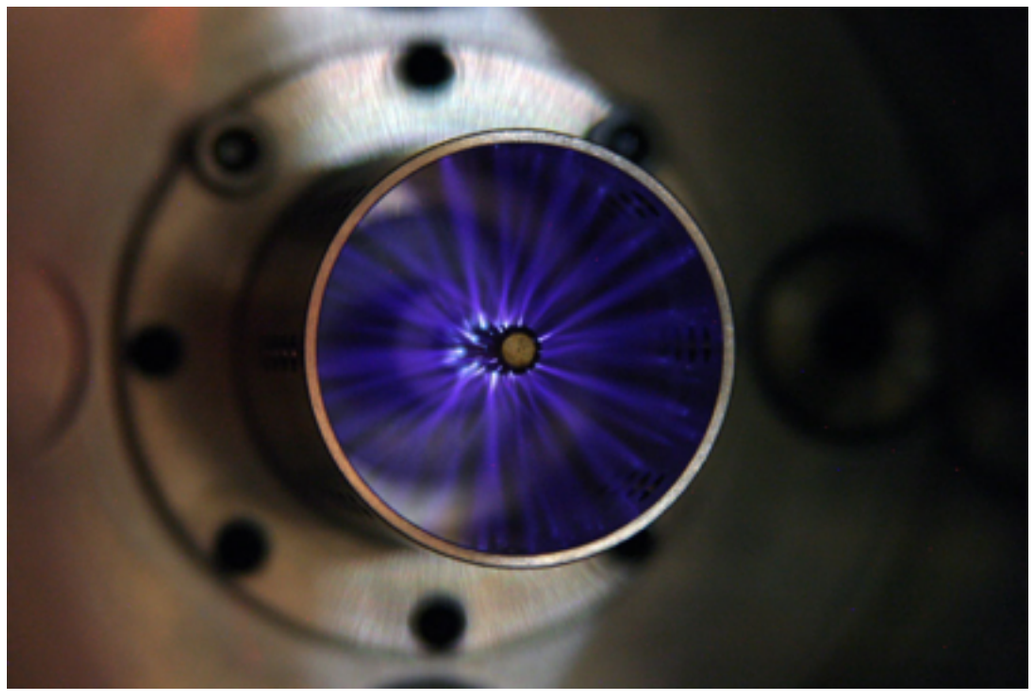
GEC
Princeton, October 1, 2013

Outline

- Motivation
- PumpKin package
- Examples
- Where to get it?

Plasma chemistry





Plasma-chemical models

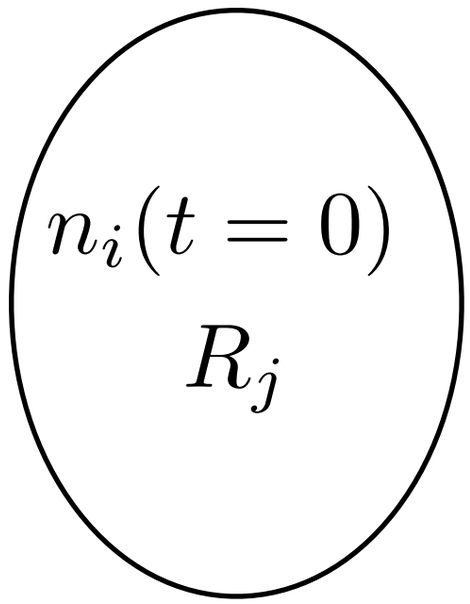
$$\frac{\partial n_i}{\partial t} = \underset{\text{gains}}{G} - \underset{\text{losses}}{L}$$

n_i concentration of the atomic and molecular neutrals, ions, electrons

G production rate of species n_i by all reactions

L destruction rate of species n_i by all reactions

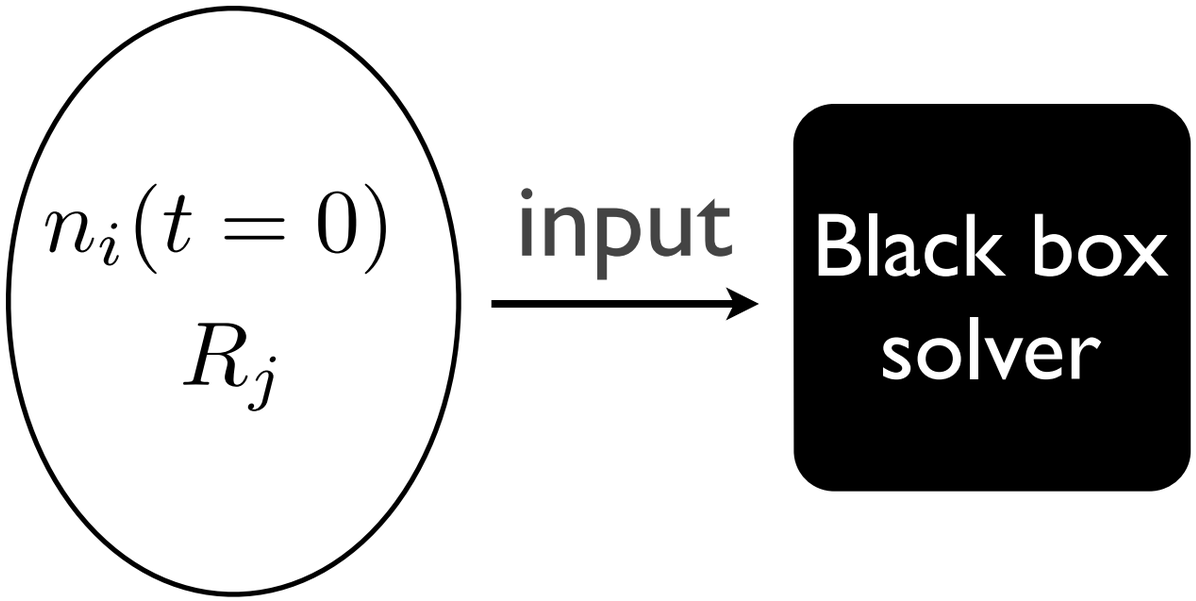
Plasma-chemical models



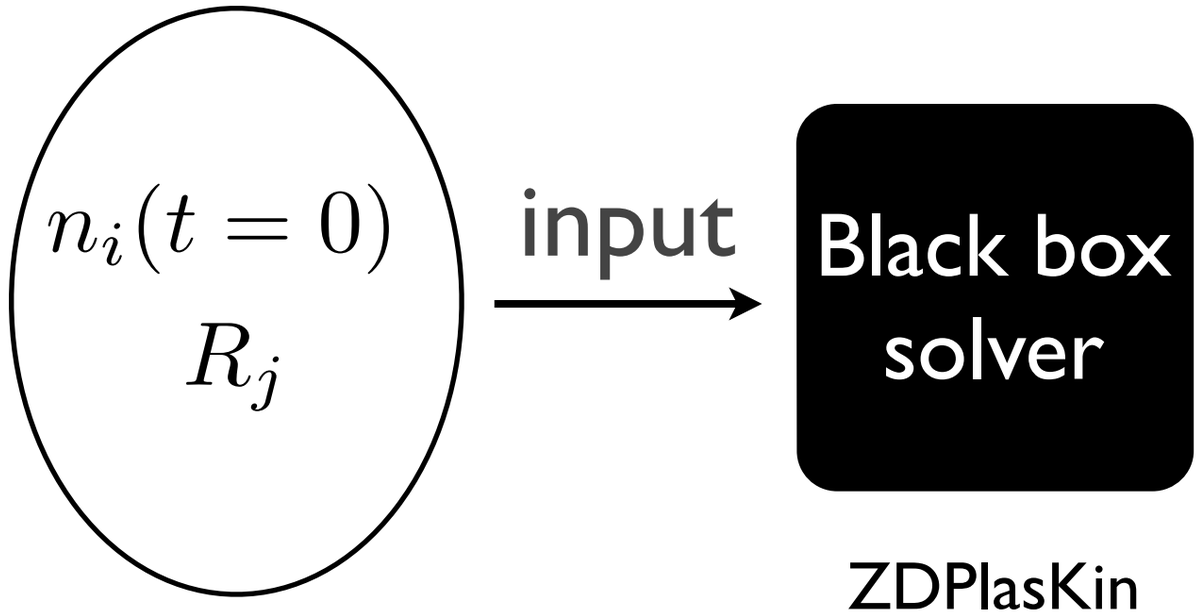
i species index

j reactions index

Plasma-chemical models



Plasma-chemical models



ZDPlasKin

Cantera

Atmos. Chem. Phys. 6, 187 (2006)

J. Phys.: Conf. Ser. 162, 012006 (2009)

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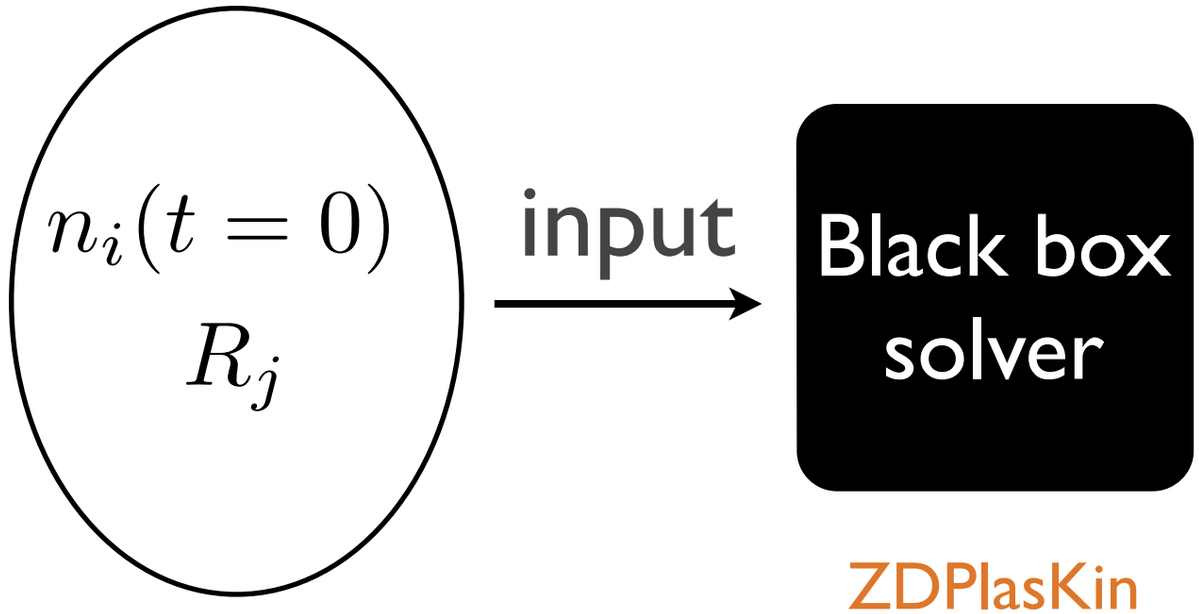
Chemkin

Plasma-chemical models



ZDPlasKin

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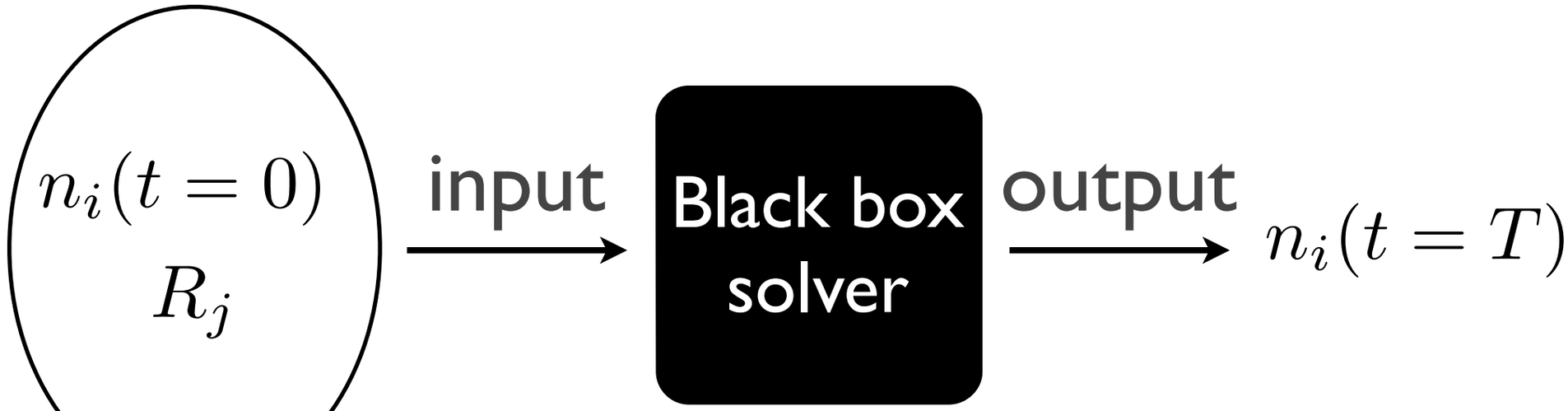
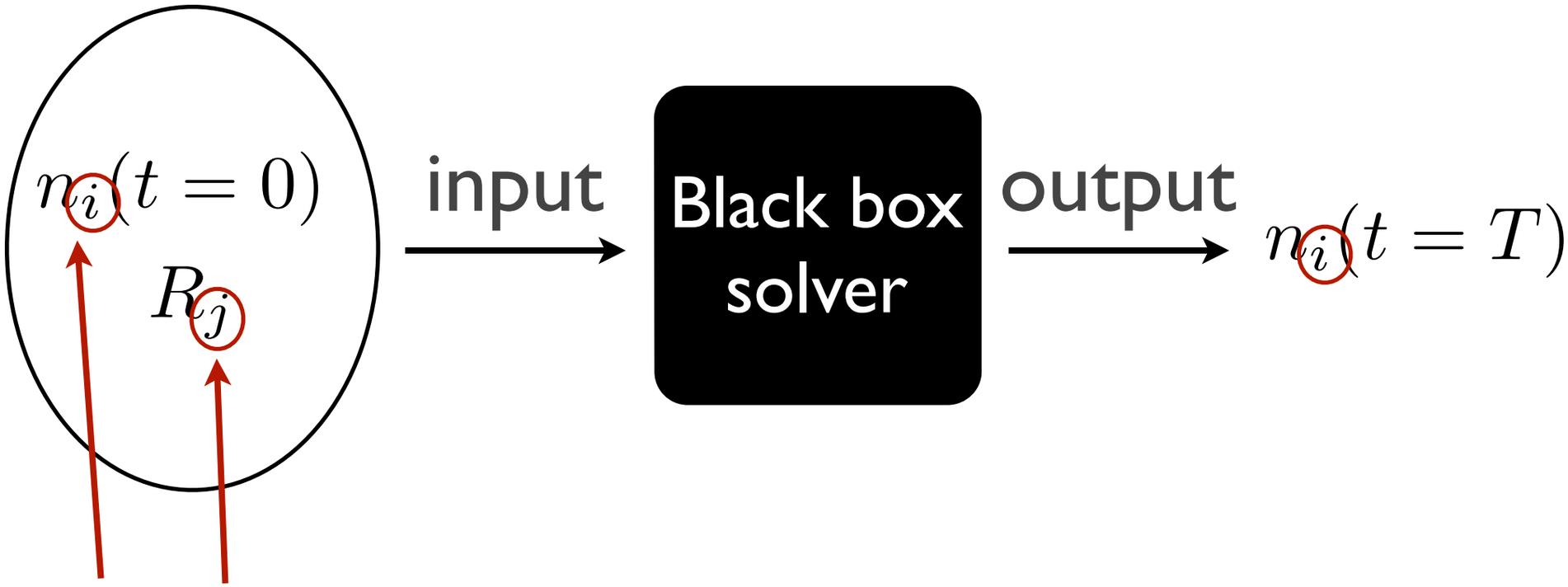
Chemkin

Plasma-chemical models

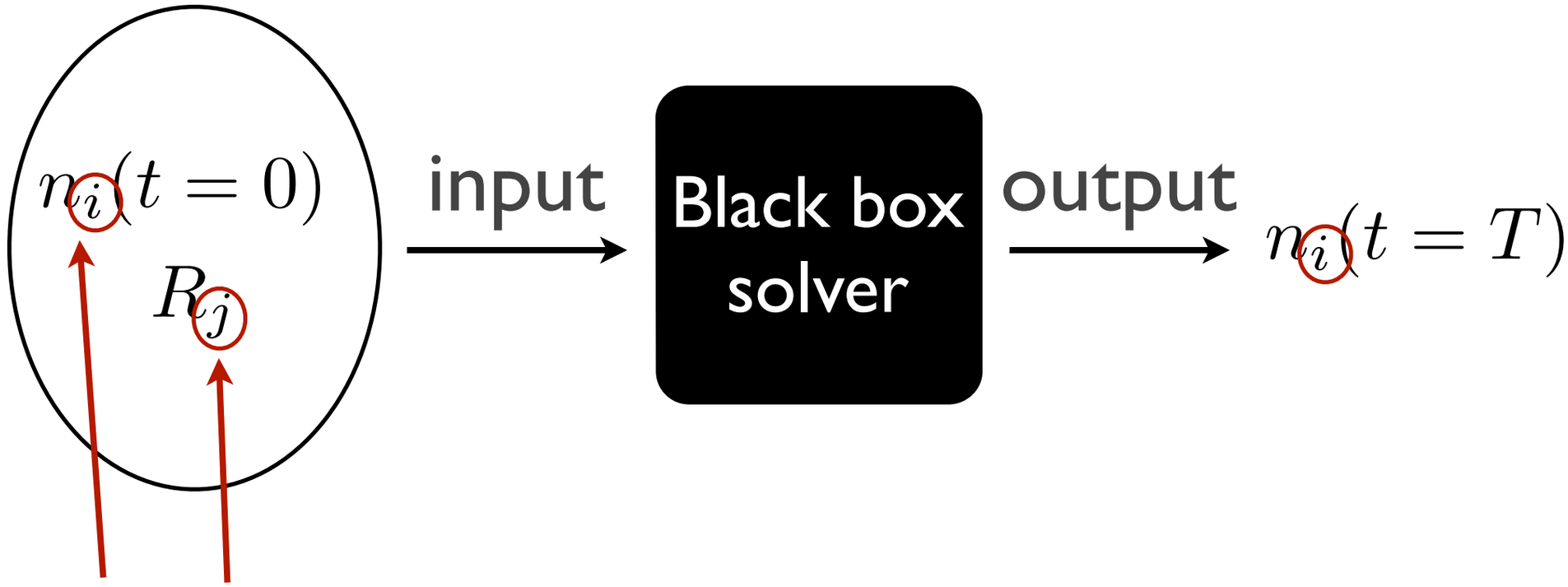


Plasma-chemical models



Can be very big!

Plasma-chemical models

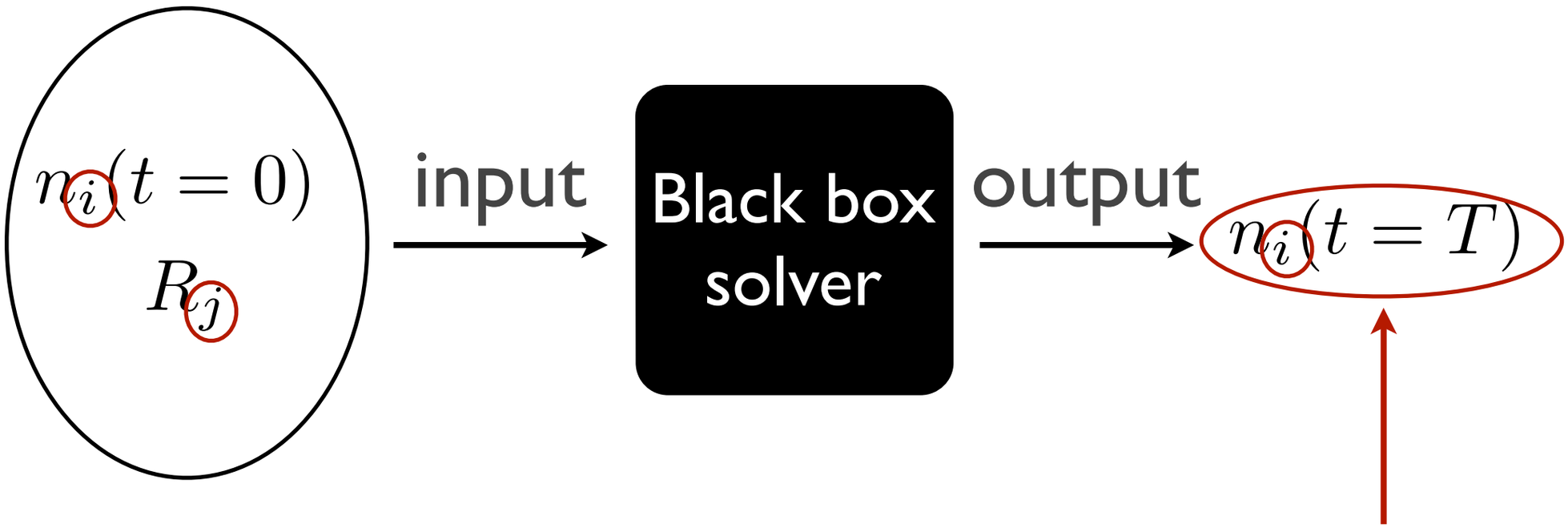


Can be very big!

- air (dry) plasma kinetics $i = 75, j = 500$
- gas giant atmosphere $i = 90, j > 2000$

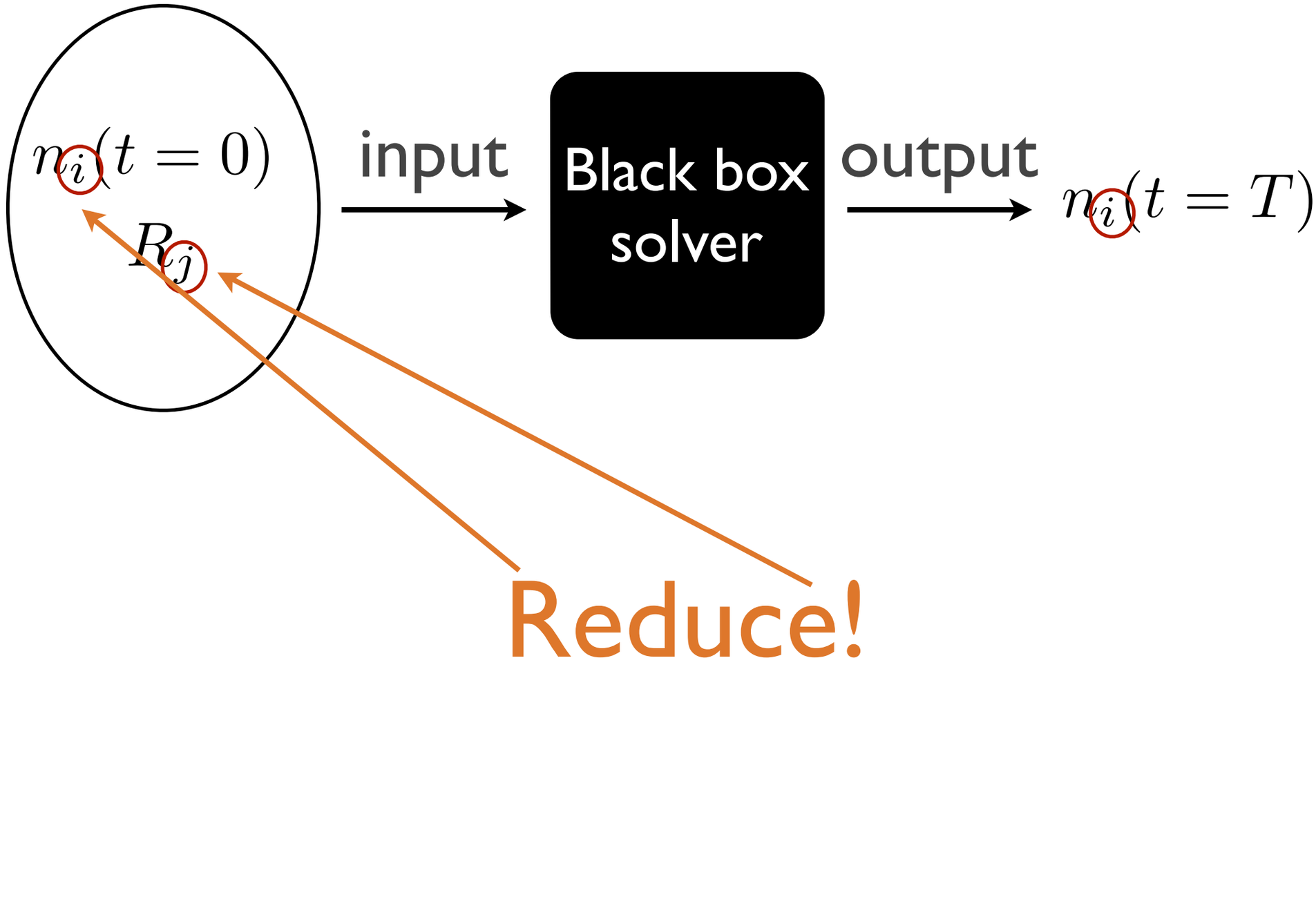
1 F.J. Gordillo-Vázquez, J Phys D Appl Phys 41, 234016 (2008)
2. C. Bilger, P. Rimmer, and C. Helling, doi:10.1093/mnras/stt1378, (2013)

Plasma-chemical models



How to understand?
What to do with this?

Plasma-chemical models



How?

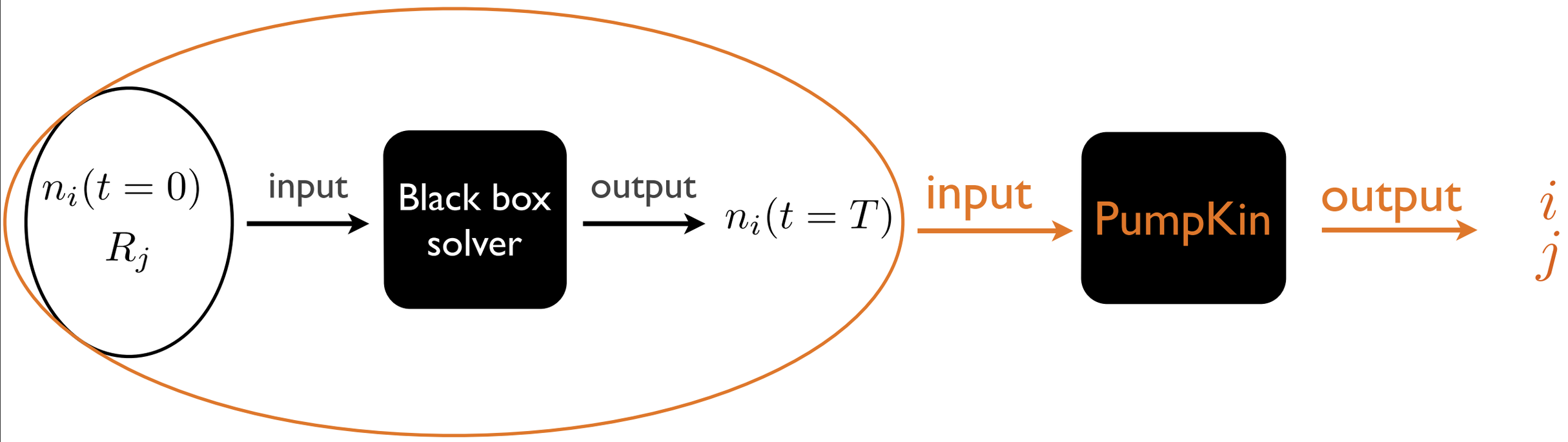
No!

PumpKin

(Pathway reduction method for plasma Kinetics)

PumpKin package

PumpKin



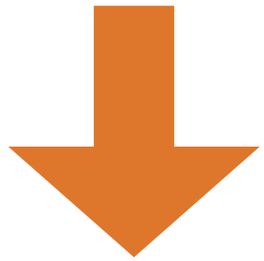
Run only once!

Input

- Stoichiometric matrix
- Concentrations of chemical species in [0,T]
- Reaction rates in [0,T]
- Time interval of interest (t_{init}, t_{end}) in [0,T]
- Species of interest S_{i^*} , if one

Output

All significant pathways [*], with rates

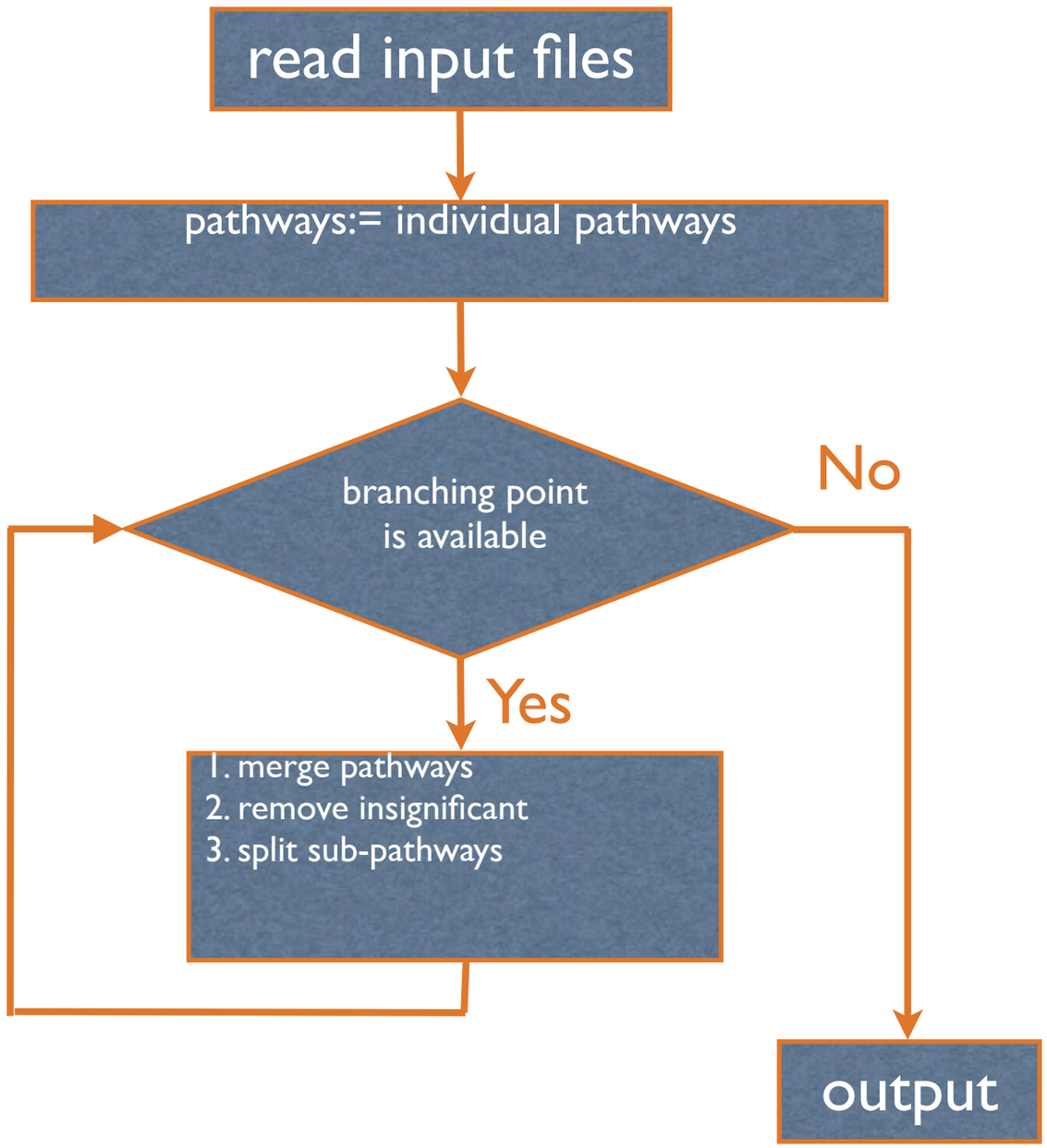


If S_i* is specified, all pathways

- producing S_i*
- destroying S_i*

[*] Pathway is a set of reactions, with a multiplicity assigned to each reaction

How does PumpKin work?



1. Schuster & Schuster, 1993
2. Lehmann, 2004: J. Atmos. Chem. 47, 45-78.

Example

Zero-dimensional kinetics using ZDPlasKin (*):

- N_2-O_2 mixture 650 reactions and 53 species
- Fixed electric field 10 kV/cm at STP
- Final time: 1ms
- Initial electron density 3.0e10 cm^{-3}

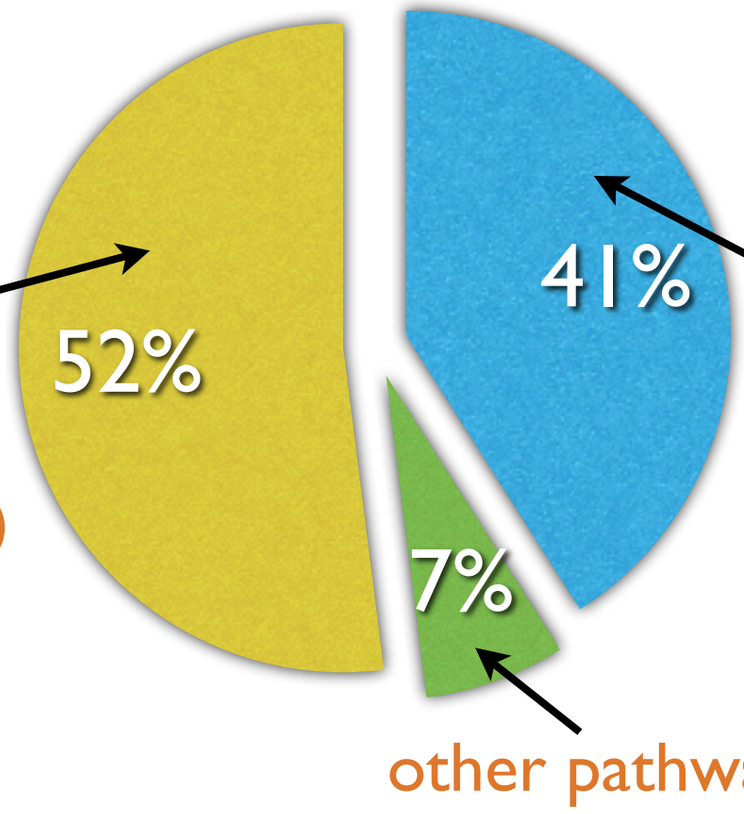
(*) S. Pancheshnyi et al., www.zdplaskin.laplace.univ-tlse.fr

Example

NO production

$$e + N_2 \rightarrow e + N + N(^2D)$$
$$N(^2D) + O_2 \rightarrow NO + O$$
$$\text{net :} \quad N_2 + O_2 \rightarrow N + O + NO,$$

(rate: 3.025e+13 mol.cm^{-3}s^{-1})



$$e + 2O_2 \rightarrow O_2^- + O_2$$
$$O_3^- + N \rightarrow NO + O_2 + e$$
$$\text{net :} \quad O_3^- + N \rightarrow O_2^- + NO + O_2.$$

(rate: 2.388e+13 mol.cm^{-3}s^{-1})

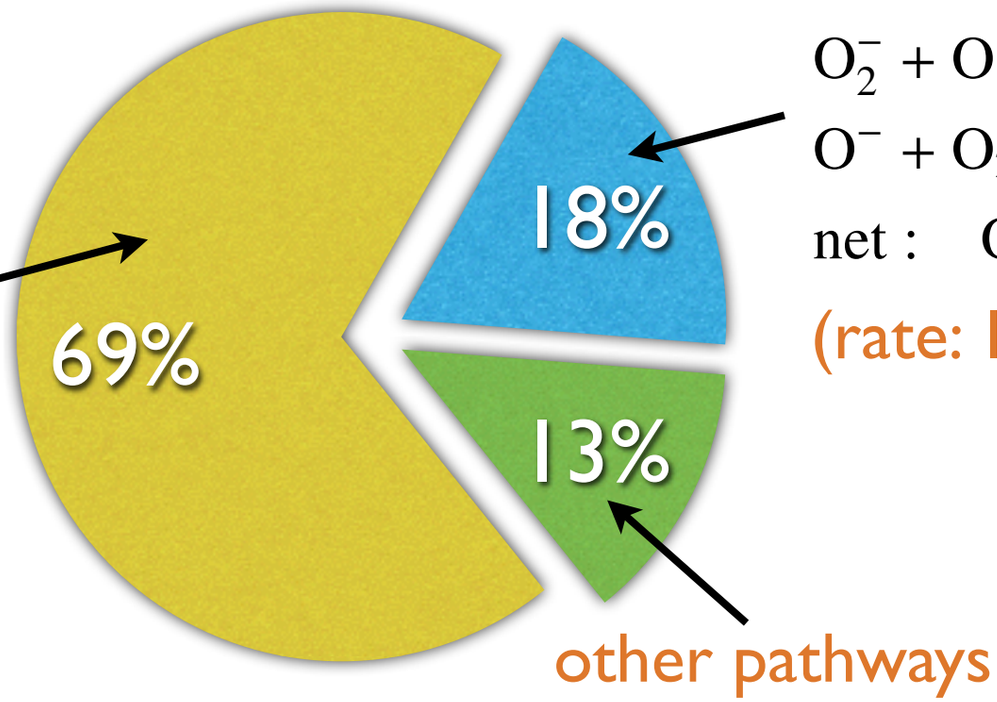
other pathways

Example

O_3^- production

$O_2^- + O_3 \rightarrow O_3^- + O_2,$

(rate: 5.337e+16 mol.cm^{-3}s^{-1})



$O_2^- + O \rightarrow O^- + O_2$

$O^- + O_2 + M \rightarrow O_3^- + M$

net : $O_2^- + O + M \rightarrow O_3^- + M,$

(rate: 1.410e+16 mol.cm^{-3}s^{-1})

Example

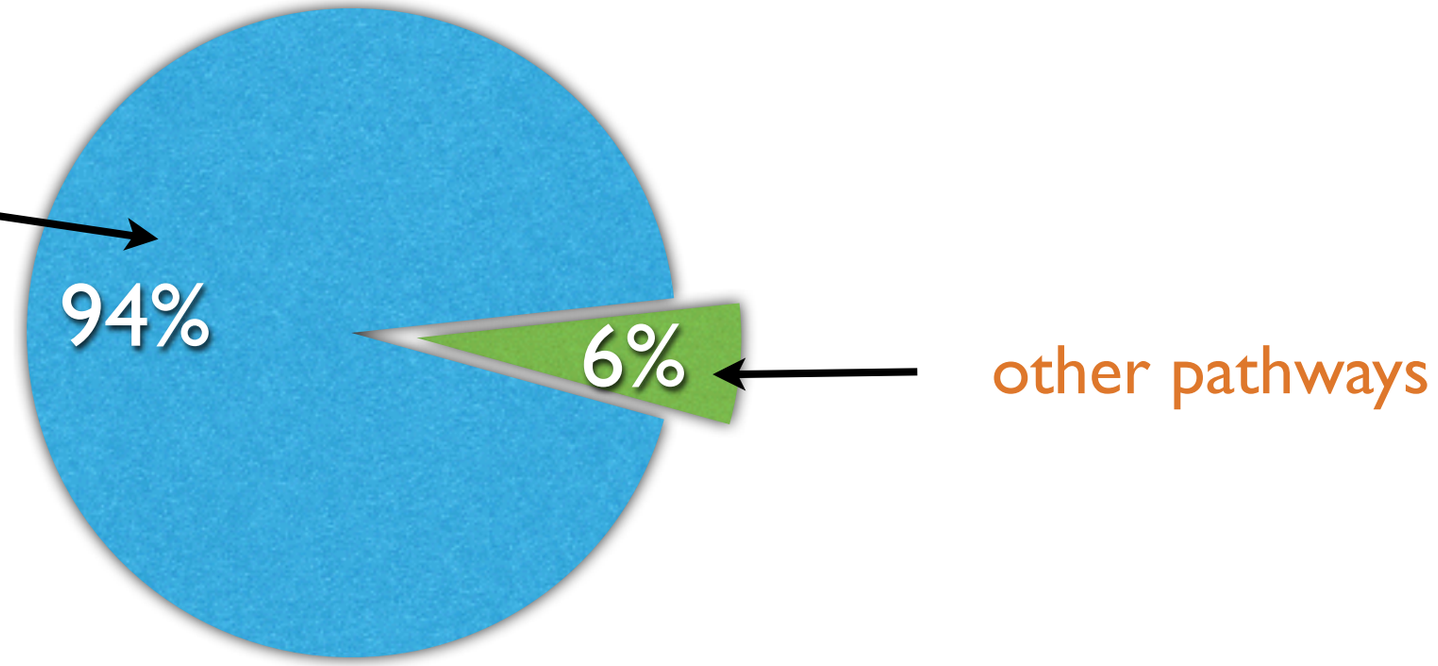
O_3^- destruction

$e + 2O_2 \rightarrow O_2^- + O_2$

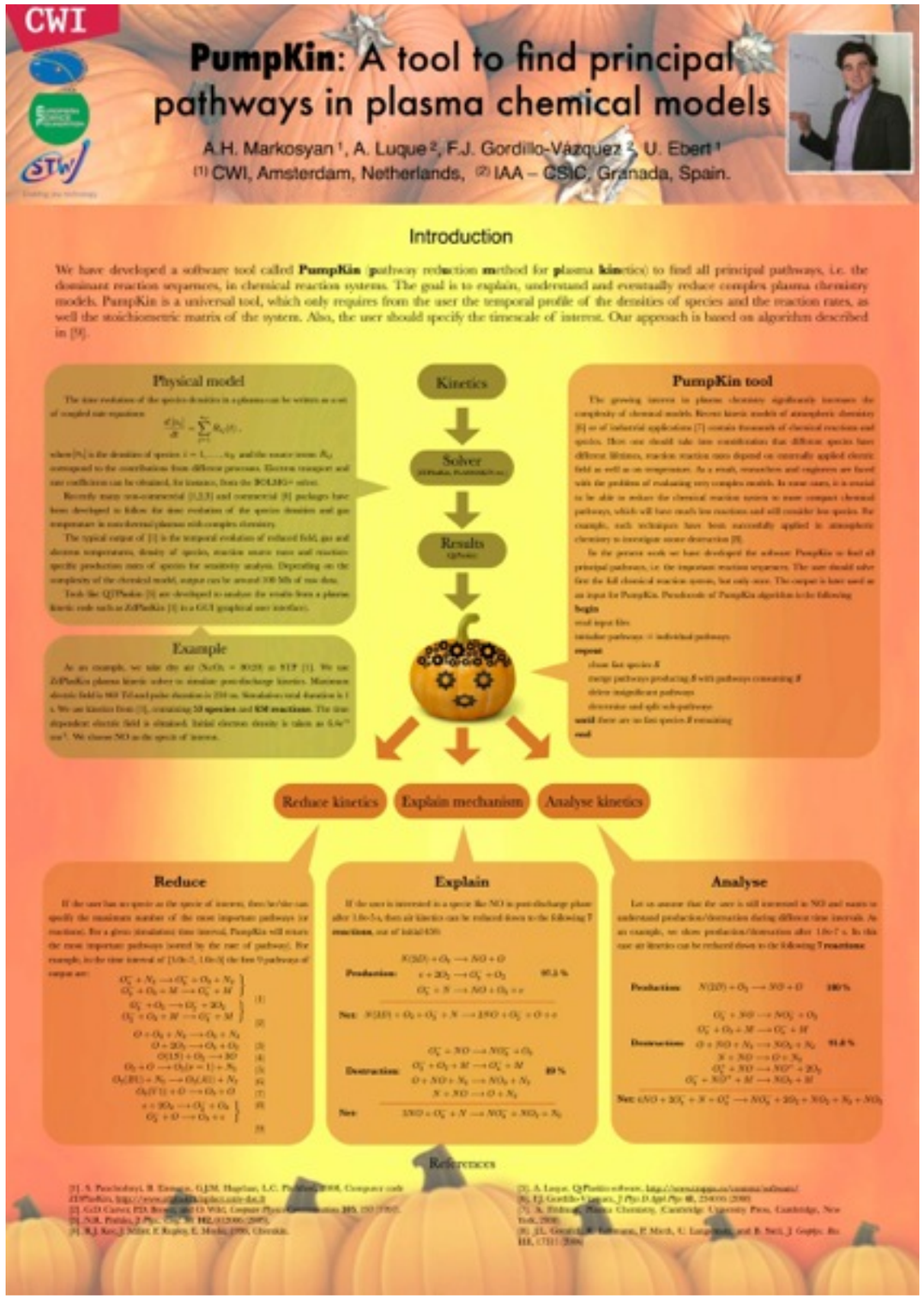
$O_3^- + O \rightarrow 2O_2 + e$

net : $O_3^- + O \rightarrow O_2^- + O_2$,

(rate: 3.097e+16 mol.cm^{-3}s^{-1})



How to get PumpKin?



How to get PumpKin?

Available soon at: www.pumpkin-tool.org

Thank you!